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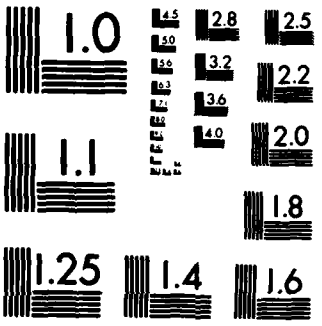

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Computer molecular dynamics studies have been carried out on the problem of attaining a fundamental understanding of shock-induced initiation of energetic materials. The studies focus on an important specific facet of this problem, namely, the energy transfer processes in crystal systems, particularly in molecular lattices. Code development for the CRAY computer during the preceding year is reviewed and the shock studies that were carried out are listed. Plans for additional studies of the underlying mechanisms of intermolecular-intramolecular energy transfer and the dynamics of intramolecular energy exchange in shock-loaded systems are presented.

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Annual Summary Report

MOLECULAR DYNAMICS STUDIES OF ENERGY TRANSFER PROCESSES IN CRYSTAL SYSTEMS

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A. Introduction

Molecular dynamics is now recognized as a very powerful technique for examining the microscopic details of a wide variety of phenomena, subject to practical computational restrictions on the length of time that one can follow the evolution of the system and on the number of particles in the system. Simply stated, molecular dynamics involves the numerical solution by computer of Newton's equations of motion for all the atoms comprising the active region of the assembly. As a result the coordinates and velocities of the particles are obtained as functions of time.

Shock-induced fast-decomposition processes are one of a wide variety of phenomena brought about by shock passage through condensed matter; such phenomena also include high-pressure polymorphic phase transitions, shock-induced polymerization, and shock-induced material syntheses. There is now an acceptance of the need to understand the microscopic details underlying shock-induced chemical and physical processes. A problem of great current interest is the attaining of a fundamental understanding of shock-induced initiation of energetic materials. Here the temporal and spatial scales involved lead us directly to considerations of a microscopic nature. Our present studies focus on an important specific facet of this problem, namely the energy transfer processes in crystal systems, particularly in molecular lattices.

By studying the dynamics of intramolecular energy exchange we can obtain information concerning the rate of energy concentration and partitioning in molecular bonds and thus obtain the probability of a given amount of vibrational energy being found in any given bond. By studying the relationship of intramolecular energy exchange to the initial energy distribution and distortion of different molecular entities after shock passage, we may be able to isolate conditions affecting the rate of vibrational energy transfer or leading to

fragmentation or bond rearrangement (i.e., "chemistry"). Localization of bond energy coupled with specific athermal processes may well be important precursors to decomposition and reaction.

B. Code Development

During the preceding contract period our molecular dynamics codes have been significantly extended to allow for a more complete treatment of molecular lattices and molecular species within these lattices. The codes now enable us to treat gases, condensed fluids, and solids, composed of atomic or molecular species, as well as mixtures of these phases. A system under study can be heated or cooled to any desired temperature prior to initiating the dynamics. Specifically, in computer program development during the contract period we have:

- developed and used codes for general heterogeneous systems. In these codes subroutines were added that enable us to evaluate for any molecular solid, liquid, or gas: the total molecular energy, the total internal energy, the energies associated with rotational or librational motion (about the center of mass), and the vibrational energy. These quantities can be evaluated for any single molecule or for any complex subset of the ensemble.

- devised and used post-processing procedures that enable us to track and plot the shock-front behavior of small propagating disturbances even when thermal motions would be several orders of magnitude larger.

- developed post-processing subroutines for Fourier analysis of the transient energy response to shock loading of an arbitrary subset of the system, thus measuring the change with time of the vibrational or torsional excitation brought about by the passage of the shock front, as well as the influence of the surrounding lattice cage on the response of the subset to shock excitation.

- written and tested a series of one-particle and two-particle statistical mechanical subroutines that enable us to calculate for a shock-loaded system such quantities as the mass density, the longitudinal component of the momentum density, the longitudinal and transversal components of the kinetic contributions to the stress, the potential energy density, the longitudinal and transverse components of the potential contributions to the stress, and various contributions to the heat flux.

- continued to develop graphics capabilities to aid in interpreting results: in addition to all the appropriate tabular data, we can produce graphs of all time-dependent properties, supplemented by computer-generated color movies.

C. Studies of Energy Transfer Processes

Shock studies were carried out during this period on water (ice), treated as a simple two-dimensional molecular structure,[1,2] and on a series of simple molecular entities embedded in monatomic host lattices.[3-5]

Our present CRAY computer codes provide us with unique resources for investigating on a microscopic scale all aspects of energy transfer from a shock front to the molecular substructure of a condensed system, as well as intermodal energy transfer between or within molecular units, or between the unit and its surrounding lattice cage. Features such as defects and grain boundaries can also be readily simulated so that the influence of such heterogeneities on energy transfer can be evaluated.

We are planning to emphasize studies of the underlying mechanisms of intermolecular-intramolecular energy transfer and the dynamics of intramolecular energy exchange. These are central issues for an understanding of shock-induced initiation. We will be exploiting the following features of our molecular dynamics codes:

- the ability to handle totally heterogeneous dynamical systems with arbitrarily complex subensembles. This allows us to explicitly include in the molecular dynamics portions of the total potential energy surface relevant to bond formation and configurational restructuring.

- the ability to look explicitly at complex molecular structures embedded in host lattices and molecular matrices. This enables us to consider in detail the pathways by which energy can be transferred from the shock front region to specific bonds or molecular units, and to delineate the transient nature of energy concentration and partitioning among the molecular bonds. The ability to treat systems of arbitrary complexity also permits an

examination of energy transfer from a propagating shock front to such structural irregularities as dislocations and grain boundaries, with the possibility of generating high-frequency modes that may excite molecular modes of the lattice.

- the developing ability to treat bonds based on molecular units rather than atoms. This will enable us to treat bond restructuring and, therefore, the associated chemistry and will enable us to examine in detail exothermic systems such as nitric oxide and nitromethane, under varying initial conditions of shock pressure, temperature, and the presence or absence of defects and structural features. Our simulations will include chemical restructuring, leading to both endothermic and exothermic reactions. The specific design of our computer codes permits early implementation of this "chemically smart" molecular dynamics.

In summary, our present codes contain novel features that represent many man-years of development and an immediately available resource enabling us to treat the initial phases of each of these problems.

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Non-equilibrium Effects Seen in Molecular Dynamics Calculations of Shock Waves in Solids (with F. E. Walker and J. R. Hardy), Proceedings of the Nato Advanced Study Institute on Non-equilibrium Cooperative Phenomena in Physics, edited by M. G. Velarde (NATO ASI Physics Series Vol. B00, Plenum Press, New York and London, 1984). (University of California Report UCRL-89884). Presentation given at the NATO Advanced Study Institute on Non-equilibrium Cooperative Phenomena in Physics, 1-11 August 1983, El Escorial (Madrid), Spain.

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Shock Compression of Two-Dimensional Computer Molecular Dynamics Water (with P. Harris and T. DeBoni), University of California Report UCRL-88973. Presentation given at the American Physical Society 1983 Topical Conference on Shock Waves in Condensed Matter, 18-21 July 1983, Santa Fe, New Mexico.

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